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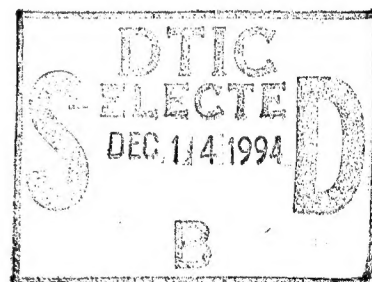
CONTINUED COMPUTATIONAL EVALUATION OF THE
FEASIBILITY OF NITRATING PRECURSORS TO $C_{12}N_{12}O_{12}$.

by

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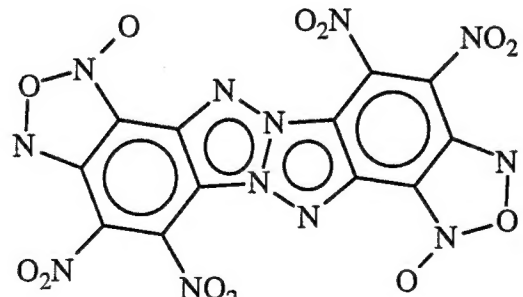


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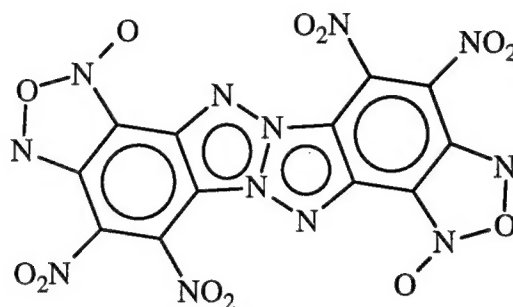
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13. ABSTRACT (Maximum 200 words) Extending the work reported in Technical Report No. 71 (October 20, 1994), we computed the average local ionization energies on the surfaces of two more possible precursors to 1. No minima were found at the positions to be nitrated, indicating that these are not favored sites for this purpose. <div style="text-align: center;">  <p style="margin-top: 10px;">1</p> </div>				
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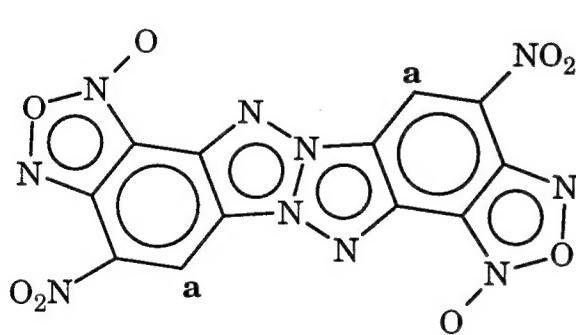
Introduction

In Technical Report No. 71 (October 20, 1994), we investigated the susceptibility to electrophilic attack involving charge transfer (as in nitration) of several possible precursors to **1**. We computed the average local ionization energies $\bar{I}_S(\mathbf{r})$ on the surfaces of **2** - **4** (Figure 1) in order to determine the ease of charge transfer at positions **a** and **b**. At the request of M. L. Trudell, we have now extended this study to include **5** and **6**. The procedure used was the same as described in the earlier report, which also discusses the definition and interpretation of $\bar{I}_S(\mathbf{r})$. The results are given in Figure 1, together with those obtained previously.

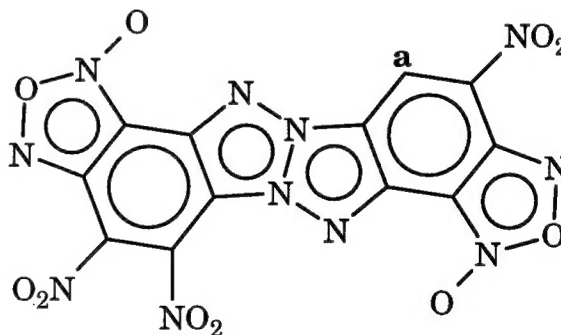


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We find no minimum in $\bar{I}_S(\mathbf{r})$ at positions **a** in **5** and **6**, which is consistent with what was observed earlier for **4**. This indicates that these are not favorable sites for charge transfer to an electrophile.



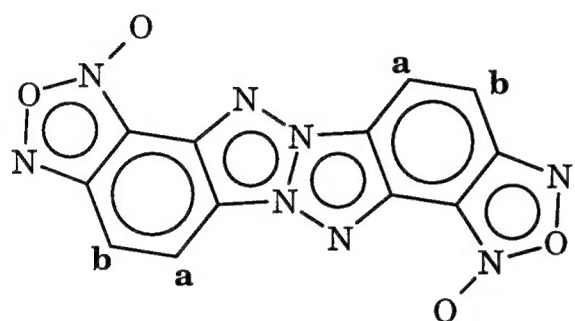
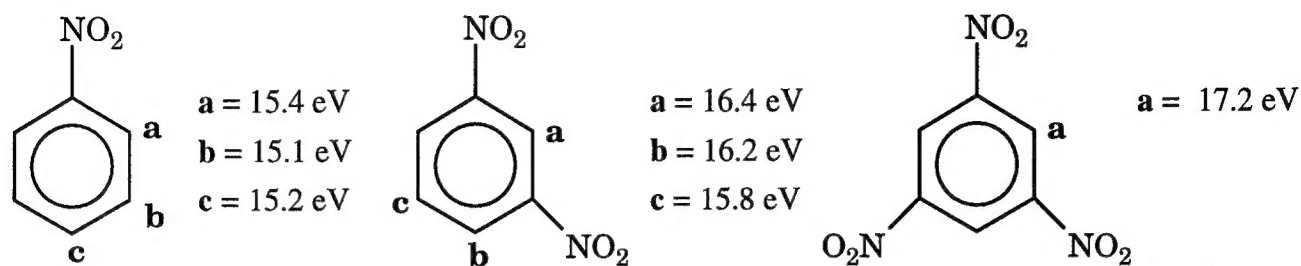
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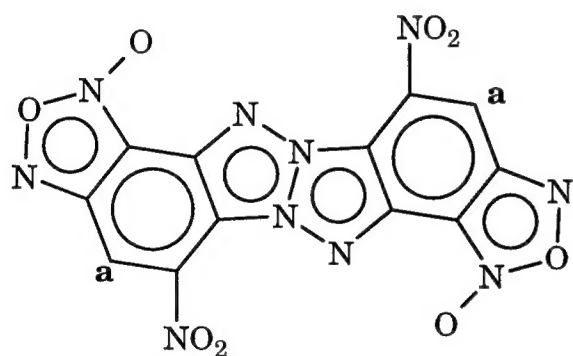
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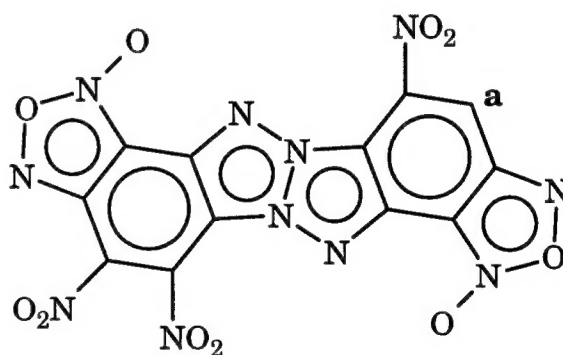
Figure 1. Some Computed (STO-5G) Minima of Average Local Ionization Energies on Molecular Surfaces



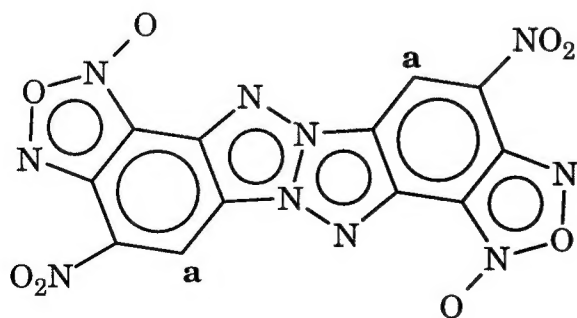
4 **a**: no minimum;
 $\bar{I}_S(\mathbf{r}) = \text{approx. } 15.9 \text{ eV.}$
b = 15.2 eV



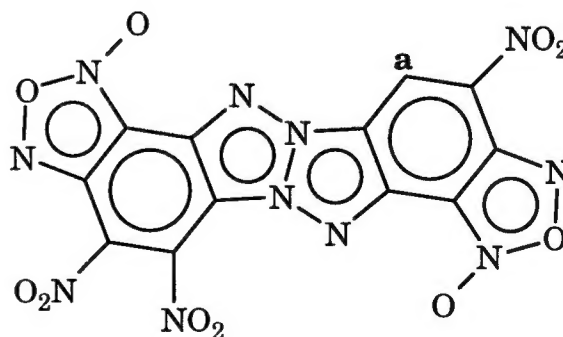
2 **a** = 16.3 eV



3 **a** = 16.6 eV



5 **a**: no minimum;
 $\bar{I}_S(\mathbf{r}) = \text{approx. } 16.8 \text{ eV.}$



6 **a**: no minimum;
 $\bar{I}_S(\mathbf{r}) = \text{approx. } 17.0 \text{ eV.}$